

A new evaluation procedure of Thermal Desorption Spectroscopy (TDS) and its application to FeCTi-alloys

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Hydrogen embrittlement (HE) is a crucial problem whenever steels with tensile strengths above 1000 MPa are used in sour environments. To improve the resistivity of such steels against HE the interaction of hydrogen with the underlying microstructure has to be investigated. Thermal Desorption Spectroscopy (TDS) is a common and well-accepted method in literature to study the trapping behavior of microstructural defects. However, the evaluation procedure of TDS spectra is not straightforward and re-trapping or the trap densities are often not considered in the analysis.

Therefore, a new numerical based interpretation method is suggested. It bases on the diffusion model for hydrogen published by Svoboda and Fischer [1]. Each trap in the model is described by a set of two parameters (trap density and binding energy). The applicability of the model were tested on TDS measurements on FeCTi-alloys [2]. By using an optimization routine, the parameters were fitted to the TDS profiles. The simulated TDS profiles agree very well with the measurements. The resulting binding energies were interpreted by using the theoretical results of Stefan and co-workers [3]. Finally, a carbon vacancy trap could be found in the high temperature range.

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[3] D. Di Stefano, R. Nazarov, T. Hickel, J. Neugebauer, M. Mrovec and C. Elsässer, *Physical Review*, 93, 184108 (2016).